

Phase Diagram of the Extended Hubbard Model with Pair Hopping Interaction

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A one-dimensional model of interacting electrons with on-site U , nearest-neighbor V , and pair-hopping interaction W is studied at half-filling using the continuum limit field theory approach. The ground state phase diagram is obtained for a wide range of coupling constants. In addition to the insulating spin- and charge-density wave phases for large U and V , respectively, we identify bond-located ordered phases corresponding to an enhanced Peierls instability in the system for $W < 0$, $|U - 2V| < |2W|$, and to a staggered magnetization located on bonds between sites for $W > 0$, $|U - 2V| < W$. The general ground state phase diagram including insulating, metallic, and superconducting phases is discussed. A transition to the η_π -superconducting phase at $|U - 2V| \ll 2t \leq W$ is briefly discussed.

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I. INTRODUCTION

The one dimensional (1D) extended Hubbard model with nearest-neighbor repulsion V , in addition to the on-site repulsion U (hereafter $U - V$ model) has been extensively studied during the last two decades as an important theoretical test-bed for studying low-dimensional strongly correlated electron systems with rich phase structures. Considerable attention has been focused on studying of the ground state (GS) phase diagram of the $U - V$ model at half-filling, using analytical studies and numerical simulations [1–15]. The sketch of the phase diagram consists of a Mott insulating phase ($U > 2|V|$) with dominating spin-density wave correlations, an insulating long-range-ordered (LRO) charge-density-wave (CDW) phase ($2V > U > 0$), and metallic phases with dominating singlet (SS) and triplet (TS) superconducting correlations. In the physically most interesting region of repulsive interactions ($U, V > 0$), the weak-coupling perturbative renormalization group studies [1,2] show that there is a continuous phase transition between SDW and CDW along the line $U = 2V$. In the strong coupling limit ($U, V \gg 1$) the SDW-CDW transition is discontinuous (first order) and the phase boundary is slightly shifted away from the line $U = 2V$ [3,4,8]. Estimates for the location of the tricritical point, where the nature of the transition changes, have ranged from $U_c \simeq 1.5$ to $U_c \simeq 5$ (and $V_c \simeq U_c/2$). [3–5,9,13] Recently increased interest towards the $U - V$ Hubbard model was triggered by Nakamura, [10–12] who found numerically that for small to intermediate values of U and V , the SDW and CDW phases are mediated by the bond-ordered charge-density-wave (BO-CDW) phase. The SDW-CDW transition splits into two separate transitions: (i) a Kosterlitz-Thouless spin gap transition from SDW to BO-CDW and (ii) a continuous transition from BO-CDW to CDW.

An analogous sequence of phase transitions in the vicinity of the $U = 2V$ line is the intrinsic feature of extended $U - V$ Hubbard models with bond-charge coupling [16,17]. The *bond located ordering* in these models is directly connected with the *site-off-diagonal nature* of the bond-charge coupling. Models of correlated electrons with bond-charge coupling have currently attracted a great interest as models showing unconventional, “kinematical” mechanisms of superconducting correlations [18–39]. Among the models with correlated “kinematics” models with pair-hopping interaction are the subject of current studies [27–39]. In this paper we consider the ground state phase diagram of extended $U - V$ Hubbard model supplemented with the pair hopping term. The Hamiltonian of the model is given by

$$\begin{aligned} \mathcal{H} = & -t \sum_{n,\sigma} (c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}) - \mu \sum_{n,\sigma} c_{n,\sigma}^\dagger c_{n,\sigma} \\ & + \frac{1}{2} U \sum_{n,\sigma} \hat{\rho}_{n,\sigma} \hat{\rho}_{n,-\sigma} + V \sum_n \hat{\rho}_n \hat{\rho}_{n+1} \\ & + W \sum_n (c_{n,\uparrow}^\dagger c_{n,\downarrow}^\dagger c_{n+1,\downarrow} c_{n+1,\uparrow} + h.c.), \end{aligned} \quad (1)$$

where $\hat{\rho}_{n,\sigma} = c_{n,\sigma}^\dagger c_{n,\sigma}$, $\hat{\rho}_n = \sum_\sigma \hat{\rho}_{n,\sigma}$, and $c_{n,\sigma}^\dagger$ ($c_{n,\sigma}$) denotes the creation (annihilation) operator for an electron with spin σ at site n . In Eq. (1), t and μ denote the hopping integral and the chemical potential respectively, with U being the on-site Coulomb-Hubbard repulsion and V the intersite interaction. W is the pair hopping interaction.

It is notable that the U , V , and W terms could be obtained from the same general tight-binding Hamiltonian [40] by focusing on a selected term of the two-particle interaction. The sign of the *Coulomb-driven* coupling constants is typically repulsive $U, V, W > 0$, and usually $W \ll U, V$. However, below we will treat these param-

eters as the effective (phenomenological) ones, assuming that they include all the possible renormalizations, and their values and signs could be arbitrary.

Interest in models with pair-hopping coupling comes from the unusual mechanisms of Cooper pairing provided by this interaction. In the absence of the on-site and nearest-neighbor couplings ($U = V = 0$), the model Eq. (1) reduces to the Penson-Kolb (PK) model [27]. The PK model is possible the simplest model which captures the essential physics of an electron system showing the η -superconductivity in the ground state. In the η -paired state, the eigenstates of the correlated electrons are constructed exclusively in terms of doublon (on-site singlet pair) creation operators [41]. We consider two different realizations of the η -paired state, constructed in terms of zero size Cooper pairs with *center-of-mass momentum equal to zero* (η_0 -pairing) and π (η_π -pairing), respectively.

In the case of an “attractive” ($W < 0$) pair-hopping interaction the PK model describes a *continuous evolution* of the usual BCS type superconducting state at $|U|, |W| \ll t$ into a local pair η_0 -superconducting state at $|W|/t \rightarrow \infty$ [28]. In the case of repulsive ($W > 0$) pair-hopping interaction, in contrast, the transition into the η_π -paired state takes place at *finite* W_c and is of *first order* (level-crossing type) [31,35,39].

In this paper we address the question, whether the pair-hopping coupling could lead to the superconducting ordering in the physically most relevant region of parameters $U, V \gg W > 0$. In this communication we present the weak-coupling ground state phase diagram of the model Eq. (1). As we show in this paper, the “attractive” ($W > 0$) pair-hopping coupling enlarges the region of coupling constant corresponding to the metallic phase with dominating SS and TS instabilities. However, in the repulsive sector of the phase diagram, along the line $U = 2V > 0$, only the insulating LRO BO-CDW phase, is realized at $|U - 2V| < |W|$. In the case of a “repulsive” ($W > 0$) pair-hopping coupling, the BO-SDW phase corresponding to a bond located staggered magnetization is together with the *CDW* the most divergent instability in the system. We also present quantitative arguments in favour of an additional phase transition at $W \simeq 4t$ from the insulating BO-SDW to the η_π -superconducting phase.

The outline of the paper is as follows: In section II we present the continuum limit bosonized version of the model. In section III we discuss the weak coupling phase diagram. Section IV is devoted to a discussion of the ground state phase diagram and a summary.

II. CONTINUUM LIMIT THEORY AND BOSONIZATION.

In this section we derive the low-energy effective field theory of the lattice model Eq. (1) at half-filling. Con-

sidering the weak-coupling case $|U|, |V|, |W| \ll t$, we linearize the spectrum and pass to the continuum limit by use of the mapping

$$a_0^{-1/2} c_{n,\sigma} \rightarrow i^n R_\sigma(x) + (-i)^n L_\sigma(x). \quad (2)$$

Here $x = na_0$, a_0 is the lattice spacing, and $R_\sigma(x)$ and $L_\sigma(x)$ describe right-moving and left-moving particles, respectively. These fields can be bosonized in a standard way [42]:

$$R_\sigma(x) = (2\pi a_0)^{-1/2} e^{i\sqrt{4\pi}\Phi_{R,\sigma}(x)}, \quad (3)$$

$$L_\sigma(x) = (2\pi a_0)^{-1/2} e^{-i\sqrt{4\pi}\Phi_{L,\sigma}(x)}, \quad (4)$$

where $\Phi_{R(L),\sigma}(x)$ are the right (left) moving Bose fields. We define $\Phi_\sigma = \Phi_{R,\sigma} + \Phi_{L,\sigma}$ and introduce linear combinations, $\varphi_c = (\Phi_\uparrow + \Phi_\downarrow)/\sqrt{2}$ and $\varphi_s = (\Phi_\uparrow - \Phi_\downarrow)/\sqrt{2}$, to describe the charge and spin degrees of freedom, respectively. Then, after a rescaling of fields and lengths, we rewrite the bosonized version of the Hamiltonian (1) in terms of two decoupled quantum SG theories, $\mathcal{H} = \mathcal{H}_c + \mathcal{H}_s$, where

$$\mathcal{H}_{c(s)} = \int dx \left\{ \frac{v_{c(s)}}{2} [(\partial_x \varphi_{c(s)})^2 + (\partial_x \vartheta_{c(s)})^2] + \frac{m_{c(s)}}{\pi a_0^2} \cos(\sqrt{8\pi K_{c(s)}} \varphi_c(x)) \right\}. \quad (5)$$

Here $\theta_{c(s)}(x)$ are the dual counterparts of the fields $\phi_{c(s)}(x)$: $\partial_x \theta_{c(s)} = \Pi_{c(s)}$ where $\Pi_{c(s)}$ is the momentum conjugate to the field $\phi_{c(s)}$. Here we have defined

$$K_c = (1 - g_c)^{-1/2} \simeq 1 + \frac{1}{2}g_c, \quad m_c = -\frac{g_u}{2\pi}, \quad (6)$$

$$K_s = (1 - g_s)^{-1/2} \simeq 1 + \frac{1}{2}g_s, \quad m_s = \frac{g_\perp}{2\pi}, \quad (7)$$

$v_{c(s)} = v_F K_{c(s)}^{-1}$ are the velocities of the charge and spin excitations, $v_F = 2ta_0(1 - W/\pi t)$, and the small dimensionless coupling constants are given by

$$g_s = g_\perp = (U - 2V + 2W)/\pi v_F, \quad (8)$$

$$g_c = -(U + 6V + 2W)/\pi v_F, \quad (9)$$

$$g_u = (U - 2V - 2W)/\pi v_F. \quad (10)$$

The relation between K_c (K_s), m_c (m_s), and g_c (g_s), g_u (g_\perp) is universal in the weak coupling limit.

In obtaining (5) the strongly irrelevant term $\sim \cos(\sqrt{8\pi K_c} \varphi_c) \cos(\sqrt{8\pi K_s} \varphi_s)$ describing umklapp scattering processes with parallel spins was omitted. The mapping of the Hamiltonian (1) onto the quantum theory of two independent charge and spin Bose fields, allows a study of the ground state phase diagram of the initial electron system using the far-infrared properties of the bosonic Hamiltonians (5). Depending on the relation between the bare coupling constants K and m the infrared

behavior of the quantum SG field exhibits two different regimes [43]:

For $|m| \leq 2(K-1)$ we are in the weak coupling regime; the effective mass $M \rightarrow 0$. The low energy (large distance) behavior of the gapless charge (spin) excitations is described by a free scalar field. The corresponding correlations show a power law decay

$$\langle e^{i\sqrt{2\pi K^*}\varphi(x)} e^{-i\sqrt{2\pi K^*}\varphi(x')} \rangle \sim |x-x'|^{-K^*}, \quad (11)$$

$$\langle e^{i\sqrt{2\pi/K^*}\theta(x)} e^{-i\sqrt{2\pi/K^*}\theta(x')} \rangle \sim |x-x'|^{-1/K^*}, \quad (12)$$

and the only parameter controlling the infrared behavior in the gapless regime is the fixed-point value of the effective coupling constants $K_{c(s)}^*$.

For $|m| > 2(K-1)$ the system scales to a strong coupling regime: Depending on the sign of the bare mass m , the effective mass $M \rightarrow \pm\infty$, which signals the crossover into a strong coupling regime and indicates the dynamical generation of a commensurability gap in the excitation spectrum. The field $\varphi_{c(s)}$ gets ordered with the vacuum expectation values [44]

$$\langle \varphi_{c(s)} \rangle = \begin{cases} \sqrt{\pi/8K_{c(s)}} & (m > 0) \\ 0 & (m < 0) \end{cases}. \quad (13)$$

The ordering of these fields determines the symmetry properties of the possible ordered ground states of the fermionic system.

Using Eqs. (8)-(10) and (13), one easily finds that there is a *gap in the spin excitation spectrum* ($M_s \rightarrow -\infty$) for

$$U - 2V + 2W < 0.$$

In this sector of coupling constants, the φ_s field gets ordered with vacuum expectation value $\langle \varphi_s \rangle = 0$. At $U - 2V + 2W \geq 0$ the spin excitations are gapless and the low-energy properties of the spin sector are described by the free Bose field system with the fixed-point value of the parameter $K_s^* = 1$.

The charge sector is gapped for

$$U > \max\{2V + 2W, -2|V|\}$$

and for

$$U < 2V + 2W \quad \text{but} \quad 2V + W > 0.$$

In the former case $M_c \rightarrow -\infty$ and the vacuum expectation value of the charge field $\langle \varphi_s \rangle = 0$, while in the latter case $M_c \rightarrow \infty$ and $\langle \varphi_s \rangle = \sqrt{\pi/8K_c}$.

In the sectors of coupling constants corresponding to the gapless charge excitation spectrum the properties of the charge degrees of freedom are described by the free Bose field

$$\mathcal{H}_c = \frac{v_c}{2} \left[K_c^* (\partial_x \varphi_c)^2 + \frac{1}{K_c^*} (\partial_x \vartheta_c)^2 \right],$$

with the fixed-point value of the parameter

$$K_c^* \simeq 1 + \sqrt{2(U+2V)(W+2V)}/\pi v_F. \quad (14)$$

Especially important is the line $U = 2V + 2W$ corresponding to the fixed-point line $m_c = 0, K_c - 1 < 0$. Here the infrared properties of the gapless charge sector are described by a free massless Bose field with the bare value of the Luttinger liquid parameter K_c .

To clarify the symmetry properties of the ground states of the system in different sectors we introduce the following set of order parameters describing the short wavelength fluctuations of the

- *site*-located charge and spin density:

$$\begin{aligned} \Delta_{CDW} &= (-1)^n \sum_{\sigma} \rho_{n,\sigma} \\ &\sim \sin(\sqrt{2\pi K_c} \varphi_c) \cos(\sqrt{2\pi K_s} \varphi_s) \end{aligned} \quad (15)$$

$$\begin{aligned} \Delta_{SDW} &= (-1)^n \sum_{\sigma} \sigma \rho_{n,\sigma} \\ &\sim \cos(\sqrt{2\pi K_c} \varphi_c) \sin(\sqrt{2\pi K_s} \varphi_s), \end{aligned} \quad (16)$$

- *bond*-located charge-density:

$$\begin{aligned} \Delta_{BO-CDW} &= (-1)^n \sum_{\sigma} (c_{n,\sigma}^{\dagger} c_{n+1,\sigma} + h.c.) \\ &\sim \cos(\sqrt{2\pi K_c} \varphi_c) \cos(\sqrt{2\pi K_s} \varphi_s) \end{aligned} \quad (17)$$

- The *bond*-located spin-density:

$$\begin{aligned} \Delta_{BO-SDW} &= (-1)^n \sum_{\sigma} \sigma (c_{n,\sigma}^{\dagger} c_{n+1,\sigma} + h.c.) \\ &\sim \sin(\sqrt{2\pi K_c} \varphi_c) \sin(\sqrt{2\pi K_s} \varphi_s). \end{aligned} \quad (18)$$

In addition we consider two superconducting order parameters corresponding to the

- singlet and triplet superconductivity:

$$\begin{aligned} \Delta_{SS}(x) &= R_{\uparrow}^{\dagger}(x) L_{\downarrow}^{\dagger}(x) - R_{\downarrow}^{\dagger}(x) L_{\uparrow}^{\dagger}(x) \\ &\sim \exp(i\sqrt{\frac{2\pi}{K_c}} \theta_c) \cos(\sqrt{2\pi K_s} \varphi_s), \end{aligned} \quad (19)$$

$$\begin{aligned} \Delta_{TS}(x) &= R_{\uparrow}^{\dagger}(x) L_{\downarrow}^{\dagger}(x) + R_{\downarrow}^{\dagger}(x) L_{\uparrow}^{\dagger}(x) \\ &\sim \exp(i\sqrt{\frac{2\pi}{K_c}} \theta_c) \sin(\sqrt{2\pi K_s} \varphi_s). \end{aligned} \quad (20)$$

III. WEAK-COUPLING PHASE DIAGRAM

With these results for the excitation spectrum and the behavior of the corresponding fields, Eqs. (11)-(13), we now discuss the *weak-coupling* ground state phase diagram of the model (1). Below we will focus on the new phases appearing in the phase-diagram due to the effect of the pair-hopping coupling. The phase diagram consists

of 5 sectors (see Fig. 1 and Fig. 2). Sectors A, B, C1, C2 are present in the phase diagram of the $U - V$ Hubbard model [7].

Sector A

- $U > \max\{2V + 2W, -2|V|\}$,

corresponds to the ordinary Mott insulating phase: The charge excitation spectrum is gapped, the spin sector is gapless. The ordering of the field φ_c with vacuum expectation value $\langle\varphi_c\rangle = 0$ leads to a suppression of the superconducting, CDW, and BO-SDW correlations. The SDW and Dimer correlations show a power-law decay at large distances

$$\begin{aligned} \langle\Delta_{SDW}(x)\Delta_{SDW}(x')\rangle &\sim \langle\Delta_{BO-CDW}(x)\Delta_{BO-CDW}(x')\rangle \\ &\sim |x - x'|^{-1}. \end{aligned} \quad (21)$$

Sector B

- $U < 2V - 2|W|$ and $2V + W > 0$

corresponds to the long-range ordered CDW insulating phase. The charge and spin excitations are gapped. The fields $\varphi_{c(s)}$ get ordered with vacuum expectation values $\langle\varphi_s\rangle = 0$ and $\langle\varphi_c\rangle = \sqrt{\pi/8K_c}$, and

$$\langle\Delta_{CDW}(x)\Delta_{CDW}(x')\rangle \sim \text{constant}. \quad (22)$$

Sector C1

- $U < \min\{2V - 2W; -2V\}$ and $2V + W < 0$

corresponds to the Singlet Superconducting (SS) phase. There a gap exists in the spin excitation spectrum and the spin field is ordered with $\langle\varphi_s\rangle = 0$. The charge excitation spectrum is gapless with the fixed point value of the parameter $K_c^* > 1$. The SDW, BO-SDW, and the TS instabilities are suppressed. The CDW, BO-SDW, and the SS instabilities show a power-law decay at large distances. However since $K_c^* > 1$ the SS instability

$$\langle\Delta_{SS}(x)\Delta_{SS}(x')\rangle \sim |x - x'|^{-1/K_c} \quad (23)$$

dominates in the ground state.

Sector C2

- $-2|V| < U < 2V - 2W$ and $2V + W < 0$

corresponds to the Luttinger liquid phase with dominating superconducting instabilities. None of the conditions of charge and spin gap is satisfied here. In this sector, the system shows the properties of a Luttinger liquid with dominating superconducting instabilities TS and SS. The singlet superconducting and triplet superconducting correlations show the same power law decay at large distances and the TS instability dominates because of the weak logarithmic corrections [7].

Finally we analyze the sectors describing the new phases. These new phases essentially appear along the

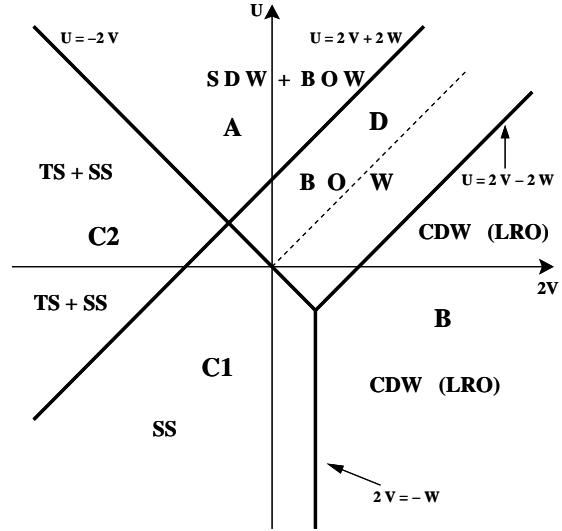


FIG. 1. The ground state phase diagram of the 1D $U - V - W$ model for the case of a half-filled band and $W < 0$. Solid lines separate different phases: A. $SDW + BOW$ - Mott insulating phase with an identical power-law decay of spin-density-wave and Peierls correlations. B. CDW (LRO) - long range ordered (LRO) charge density wave phase; C1. Singlet superconducting phase. C2. Metallic phase with dominating singlet and triplet superconducting correlations. D. LRO dimerized (Peierls) phase.

SDW - CDW transition line $U = 2V > 0$ of the $U - V$ Hubbard model. In the weak-coupling limit, the transition from the Mott insulating phase at $U > 2V$ to the CDW insulator at $U < 2V$ is mediated by the Luttinger liquid phase with gapless spin and charge excitations. At $U = 2V$ the Mott insulator charge gap closes and at $U - 2V < 0$ the charge and the spin gap opens simultaneously. In the very presence of the pair-hopping interaction, the SDW - CDW transition splits into two transitions: Along the line $U = 2V - 2W$ the spin gap opens, while at $U = 2V + 2W$ the Mott insulator charge gap closes, and for $U < 2V + 2W$ the CDW charge gap opens. In the case of an attractive pair-hopping interaction $W < 0$ (Fig. 1) the spin gap opens in the presence of a Mott insulator charge gap. Therefore, in sector D

- $|U - 2V| < 2|W|$, $2V + W > 0$,

the charge and spin channels are gapped and both, charge and spin fields are ordered, $\langle\varphi_c\rangle = \langle\varphi_s\rangle = 0$. In this case the long-range ordered BOW phase

$$\langle\Delta_{BO-CDW}(x)\Delta_{BO-CDW}(x')\rangle \sim \text{constant} \quad (24)$$

is realized in the ground state.

In the case of a repulsive pair-hopping coupling $W > 0$ (Fig. 2), the transition within the charge degrees of freedom, takes place before the spin gap opens. Therefore, in sector D1

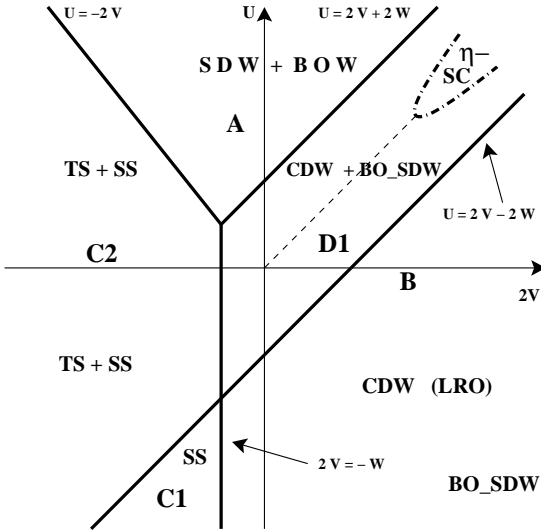


FIG. 2. The ground state phase diagram of the 1D $U - V - W$ model for the case of a half-filled band and $W > 0$. The dot-dashed line marks a transition to the η_π -superconducting phase.

- $|U - 2V| < 2|W|$ and $U + 2V > 0$,

the generation of a gap in the charge excitation spectrum, accompanied by the ordering of the field φ_c with vacuum expectation value $\langle \varphi_c \rangle = \sqrt{\pi/8K_c}$, leads to a suppression of the superconducting, SDW, and BO-CDW ordering. The CDW and BO-SDW correlations show a power-law decay at large distances

$$\begin{aligned} \langle \Delta_{CDW}(x) \Delta_{CDW}(x') \rangle &\sim \langle \Delta_{BO-SDW}(x) \Delta_{BO-SDW}(x') \rangle \\ &\sim |x - x'|^{-1}. \end{aligned} \quad (25)$$

Therefore, this sector of the phase diagram corresponds to the insulating phase with coexisting CDW and BO-SDW instabilities.

Let us now discuss the η_π -superconducting phase. In models with “kinematical” mechanisms of Cooper pairing, transition to an η -paired phase is typically the *finite-bandwidth phenomenon* [19,22–24]. In the case of pair-hopping interaction, the transition point is determined by the competition between the single-electron and doublon delocalization energies. After the transition the contribution of the one-electron hopping term to the ground state energy almost vanishes and the ground state energy is determined by the created strongly correlated two-particle η_π -pair band [35,39]. Simultaneously, after the transition the spin gap opens in the system while the charge gap (at half-filling) closes [31]. In the case of the PK model the transition point $W_c(U = V = 0) \simeq 1.8t$ [35], while in the case of the on-site Hubbard repulsion, $W_c(V = 0) \simeq 1.8t + \alpha U$, where α is of the order of unity [39]. In both cases the insulating CDW

+(BO-SDW) phase is unstable toward transition to the η_π -superconducting state [36,37,39]. Due to the finite-bandwidth nature of the transition to a η_π -paired state, it could not be consistently studied within the continuum-limit (infinite band) approach. Nevertheless, the existence of a transition is clearly traced in the additive renormalization of the Fermi velocity (bandwidth) by the pair-hopping term $v_F = 2ta_0(1 - W/\pi t)$. In the narrow stripe along the frustration line $|U - 2V| \ll W$, the effects of the on-site and nearest-neighbor repulsion cancel each other. The dimensionless coupling constants controlling the spin degrees of freedom (8) are exactly the same as in the case of the PK model. Therefore we conclude that along the frustration line $U = 2V$ an additional phase transition with increasing W from the BO-SDW to the η_π -superconducting takes place with $W_c \simeq W_c(U = V = 0) \simeq 2t$. Numerical studies of this sector of the phase diagram are currently in progress and will be published elsewhere.

IV. DISCUSSION AND SUMMARY

To summarize, we have presented the weak-coupling ground state phase diagram for 1D extended $U - V$ Hubbard with pair-hopping in the case of a half-filled band. We have shown that the model has a very rich phase diagram which includes the singlet-superconducting phase, a metallic phase with dominating SS and TS instabilities and four different insulating phases corresponding to the Mott antiferromagnet, the CDW insulator, the bond-ordered CDW and the bond-ordered SDW phase. In addition, we argued for the existence of a phase transition to the η_π -superconducting phase within the narrow stripe at $|U - 2V| \ll 2t \leq W$.

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